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MULTISCALE MODELLING APPROACH FOR A FUNGAL BIOFILTER UNIT FOR THE HYDROPHOBIC ABATEMENT OF VOLATILE ORGANIC COMPOUNDS

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Abstract

Currently, biofiltration has become a viable and potential alternative for the treatment of airstreams with low concentrations of hydrophobic volatile organic compounds (VOCs), which can employ to this end, diverse microorganisms (such as, bacteria, fungal or microbial consortia, etc.) growing a biofilm. Usually, the design, analysis and scale-up of this kind of units have been mainly done via experimental approach, which can be costly in terms of time and resources. Therefore, the objective of this work is to introduce mathematical model for the prediction and simulation of a fungal biofilter through a systematic mathematical multiscale modeling approach, thereby describing the involved phenomena at different time and dimension levels of abstraction (from macroscale to microscale level).

INTRODUCTION

Biofiltration is a viable and potentially alternative for the treatment of airstreams with low concentrations of VOCs. It utilizes a microbial population immobilized in the biofilm grown on a solid support to degrade organic pollutants in waste gas streams (bacteria, fungal or microbial consortia).

The hydrophobic VOCs biofiltration using filamentous fungi has been studied due to its several advantages over bacterial biofilters: a) fungi are more resistant to acid and dry conditions than bacteria, which is a helpful property when operating biofilters, b) their capacity to colonize empty space with the aerial hyphae and c) to penetrate the solid support increasing the availability of nutrients (Qi et al., 2002, Vergara-Fernández et al., 2006, 2008; van Groenestijn et al., 2001). On the other hand, the fungal biofilters have a number of disadvantages as: a) a slower growth than bacteria, b) increased pressure drop, c) possible production and emission of spores d) and possible obstruction of air passage and channeling (Prenafeta-Boldú et al., 2006; Vergara-Fernández et al., 2011).

Ottengraff and van den Oever (1983) presented the first VOCs biotreatment in biofilters with a diffusion and biodegradation model of pollutants in biofilms. While several models, with increased degree of complexity were reported thereafter (Devinny et al., 1999), the original description often has been used to represent biofiltration data (Pineda et al., 2000). The modeling of these systems involve physical and biochemical phenomena, including fluid flow and diffusion properties of microbial communities and packing material, prediction of active area and biofilm thickness (Alonso et al., 2000; Bibeau et al., 2000).

For the case of modeling fungal biofilters, Spigno et al. (2003) and Spigno and De Faveri (2005) performed a simple model of axial dispersion in steady state to evaluate the *n*-hexane elimination in a biofilter using the fungus *Aspergillus niger*. This model performs the same considerations that the models used for microbial consortia and bacterial biofilter, working with a homogeneous biofilm and constant biomass. An improvement including partition coefficient in the fungi, biofilm thickness, superficial area and effective diffusivity has been recently presented by Arriaga and Revah (2009).

Vergara-Fernández et al. (2008) developed a mathematical model considering the physical and biological phenomena in a fungal biofilter. The biofilter is mathematically described and the main physical (mass transfer, partition and transport area), kinetic data (substrate inhibition and affinity, growth and degradation rates and maintenance coefficient), and morphological parameters of aerial hyphae were obtained by independent experiments for model verification. The model proposed in this study (Vergara-Fernández et al., 2008) describes the increase in the transport area by the growth of the filamentous cylindrical mycelia and its relation with *n*-hexane elimination in quasi-stationary state in a biofilter.

Morales-Rodriguez (2009) proposed a systematic manner for solving mathematical models describing phenomena at different levels of abstraction, which is well known as multiscale modeling approach. The study focused on the development of products (high-value structured/special chemicals) and processes through the use of mathematical models. The systematic methodology for solving and understanding involving multiscale mathematical models, has been used for the fungal biofilter unit.

Thus, the objective of this work is to describe the multiscale mathematical model for the fungal biofilter on the hydrophobic abatement of organic volatile compounds. The mathematical model also introduces the effect of the moisture content and growth of filamentous fungi for the degradation of hydrophobic VOCs in biofilters. The biological system under study was the removal of gaseous *n*-pentane by *Fusarium solani* B1.

MULTISCALE MODELLING OF THE FUNGAL BIOFILTER: REPRESENTATION AND MATHEMATICAL MODEL.

The multiscale representation for the fungal biofilter for the VOC's is illustrated in Figure 1, which includes three different levels of abstractions, macro, meso and micro.

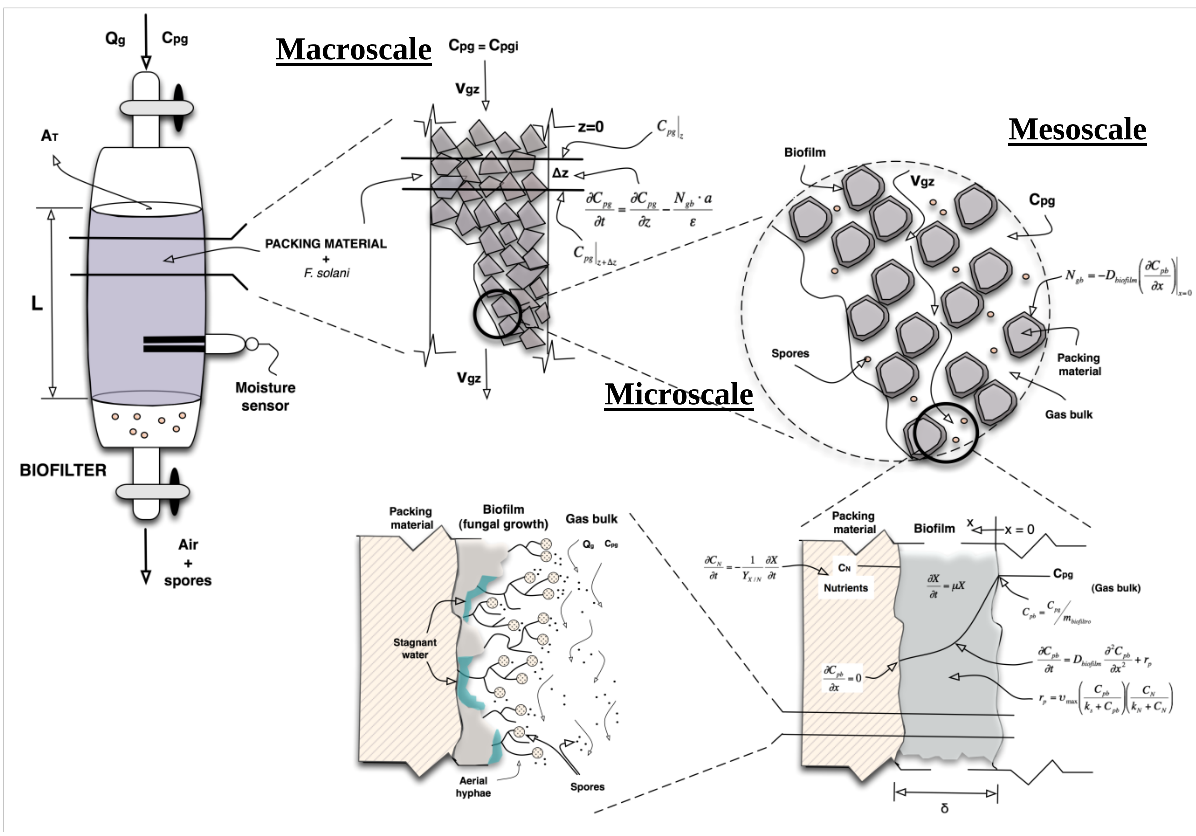

Figure 1 Multiscale modelling representation for the fungal biofilter reactor.

The mathematical model (Table 1) describes the main physical characteristics in the reactor. The macroscale level includes the equation which describes different phenomena at reactor level. The mesoscale and microscale describes the behavior at biofilm scale, the equations consist of mainly the kinetics for the bioreactor (such as, affinity constant, growth and degradation rate of substrate and nutrients, and cellular yield), besides the introduction of the effect of moisture content of packing material and elimination capacity.

Table 1. Multiscale dynamic mathematical model for fungal biofilter for the abatement of VOC's.

Scale	Description	Equation	
Macro	Elimination Capacity	$EC = \frac{Q_g}{V_r}\left(C_{pgi} - C_{pg}\right)$	Eq. (1)
	Masss balance in the biofilter	$\frac{\partial C_{pg}}{\partial t} = \upsilon_z \frac{\partial C_{pg}}{\partial z} - \frac{N_{gb} \cdot a}{\varepsilon}$	Eq. (2)
	n-pentane inlet load	$L = \frac{Q_g}{V_r} C_{pgi}$	Eq. (3)
	Interstitial gas velocity	$\upsilon_z = \frac{Q_g}{A_T \varepsilon}$	Eq. (4)
	Volumetric maximum growth rate	$\upsilon_{\max} = \mu_{\max} \frac{X}{Y_{X/S}}$	Eq. (5)
Meso	Specific mass flux from the gas to the biofilm	$N_{gb} = -D_{biofilm}\left(\frac{\partial C_{pb}}{\partial x}\right)\Big\vert_{x=0}$	Eq. (6)
Micro	Masss balance in the biofilm	$\frac{\partial C_{pb}}{\partial t} = D_{biofilm} \frac{\partial^2 C_{pb}}{\partial x^2} - r_p$	Eq. (7)
	Kinetic for fungal growth	$r_p = \upsilon_{\max}\left(\frac{C_{pb}}{k_s + C_{pb}}\right)\left(\frac{C_N}{k_N + C_N}\right)$	Eq. (8)
	Kinetic for biomass growth	$\mu = \mu_{\max}\left(\frac{C_{pb}}{k_s + C_{pb}}\right)\left(\frac{C_N}{k_N + C_N}\right)$	Eq. (9)
	Mass balance for cell growth	$\frac{\partial X}{\partial t} = \mu X$	Eq. (10)
	Mass balance nutrients consumption	$\frac{\partial C_N}{\partial t} = -\frac{1}{Y_{X/N}} \frac{\partial X}{\partial t}$	Eq. (11)
	effect of moisture content	$\mu_{\max} = k_1 x_w e^{-k_2 x_w}$	Eq. (12)
	Effect of moisture content over partition coefficient	$\frac{1}{m_{biofilter}} = \frac{x_{biomass}}{m_{biomass}} + \frac{x_w}{m_{p/w}}$	Eq. (13)
	Diffusion coefficients in the biofilm as function of the cell growth	$f(X) = \frac{D_{biofilm}}{D_{water}} = 1 - \frac{0.43 \cdot X^{0.92}}{11.19 + 0.27 \cdot X^{0.99}}$	Eq. (14)

SIMULATIONS FOR THE MULTISCALE MATHEMATICAL MODEL OF THE FUNGAL BIOFILTER

The simulation of the multiscale mathematical model for the fungal biofilter, was performed part of the set of the equations illustrated in Table 1. Two different approaches were done:

- Single Multiscale approach (SS): Solution of the model considering a Continuous stirred-tank reactor.
- Multiscale approach (MS): Solution of the model considering the spatial behaviour along the reactor in the time.

For SS, a simulation of the mathematical model considering a CSTR was performed using equations of Table 1 with exception of Equations (2), (6), (7). The mass balance for pentane in the biofilter to substitute Equation (2) was used as following:

$$\frac{\partial C_{pg}}{\partial t} = \frac{Q_{in} C_{pg}^{in} - Q_{out} C_{pg}}{V_{reactor}} - r_p \qquad \text{Eq. (15)}$$

C_{pb} in Equations (8) and (9) were changed by C_{pg} since biofilm Equation (7) was not used at all in the solution of the mathematical model.

For MS approach, the solution was done using the Equations in Table 1. The behaviour of the biofilm was not considered, thereby, Equations (6) and (7) were no solved. As explained above, C_{pb} was replaced by C_{pg} in Equations (8) and (9). The last term on the right hand side of Eq. (2) was substituted by r_p. The solution of the MS dynamic mathematical model was done discretizing the differential equation along the length of the reactor.

The dynamic simulation of the MS mathematical model was done using Matlab.

The solution of the different approaches is illustrated in Figure 2 for: Single Multiscale solution (CSTR, see Figure 2.a); Multiscale approach using two nodes (Figure 2.b) and fifty nodes (Figure 2.c). The Multiscale solutions provides more information as the number of nodes is increased, for example, when it is used more number of nodes it is possible to get more information in along the reactor. The different lines in Figure 2.c represent pentane concentration at different position in the reactor. For Figure 2.b when two nodes are used for the diacretization along the reactor, the plot shows less information if compare when fifty nodes are used. The solution for single multiscale (Figure 2.a) shows the profile of the biofilter in the time, since the CSTR model assumes that the concentration inside the reactor is equal, the results of the model just provided on single curve.

Another of the differences can found when pentane concentration reaches a steady state profile, meaning that the nutrient in the reactor has been totally consumed (Figure 2.a-c). The same trend can be seen for elimination capacity (Figure 2.d), which becomes zero when no nutrient is present in the reactor. Some differences in the time when elimination capacity is zero are also observed for the different employed approaches, meaning that the precision of the model is improved as the complexity of the model is increased. Comparing these results with the experimental data, it is possible to observe that the model is able to predict the time when elimination capacity is equal to zero.

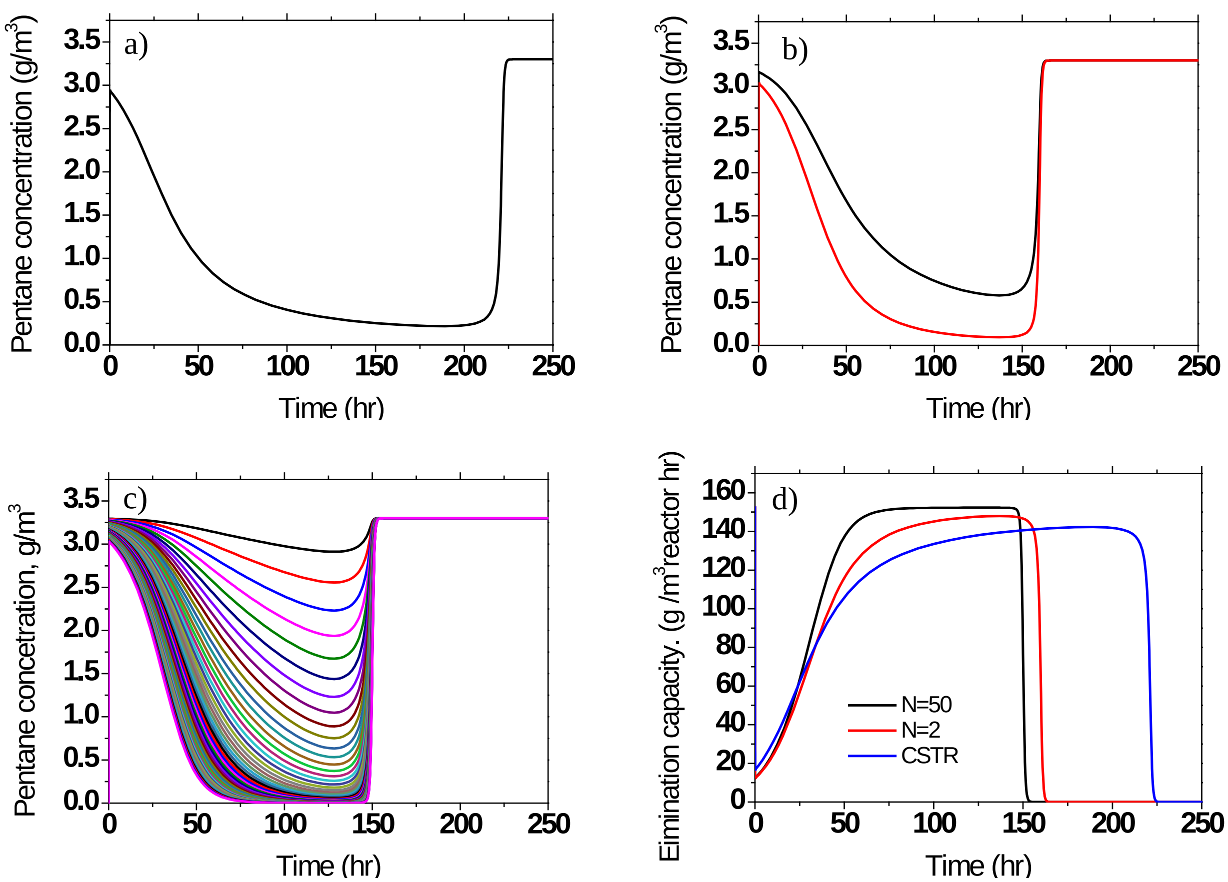

Figure 2. Mathematical model simulation the analyzed approaches: a) SS, CSTR solution, b) MS using two nodes, c). MS using Fifty nodes. d) Elimination capacity in the biofilter for the different approaches.

CONCLUDING REMARKS

This study has presented the multiscale dynamic mathematical model for a fungal biofilter unit in the abatement of VOC's. The advantages of the multiscale modelling approach was also presented and analyzed using some simulations of the mathematical model. The results illustrated that model accuracy is increased as the complexity or number of mathematical equations is also increased. Similarly as the amount of information that can be obtained when multiscale modelling approach is employed, for instance, if the number of nodes is creased, the solution of the mathematical model would be able to provide a local concentration along the reactor. The results have been compared with experimental data obtained from the lab.

For future work, the equations for predicting the behaviour in the biofilm will be added to the set of partial diferential equations. Moreover, the effect of sporulation will be introduced in the model to predict this important phenomenon that is present when the biofilter is in operation.

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